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* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *
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NEWS  1            Web Page for STN Seminar Schedule - N. America
NEWS  2   DEC 01   ChemPort single article sales feature unavailable
NEWS  3   FEB 02   Simultaneous left and right truncation (SLART) added
                   for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS  4   FEB 02   GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS  5   FEB 06   Patent sequence location (PSL) data added to USGENE
NEWS  6   FEB 10   COMPENDEX reloaded and enhanced
NEWS  7   FEB 11   WTEXTILES reloaded and enhanced
NEWS  8   FEB 19   New patent-examiner citations in 300,000 CA/CAplus
                   patent records provide insights into related prior
                   art
NEWS  9   FEB 19   Increase the precision of your patent queries -- use
                   terms from the IPC Thesaurus, Version 2009.01
NEWS 10   FEB 23   Several formats for image display and print options
                   discontinued in USPATFULL and USPAT2
NEWS 11   FEB 23   MEDLINE now offers more precise author group fields
                   and 2009 MeSH terms
NEWS 12   FEB 23   TOXCENTER updates mirror those of MEDLINE - more
                   precise author group fields and 2009 MeSH terms
NEWS 13   FEB 23   Three million new patent records blast AEROSPACE into
                   STN patent clusters
NEWS 14   FEB 25   USGENE enhanced with patent family and legal status
                   display data from INPADOCDB
NEWS 15   MAR 06   INPADOCDB and INPAFAMDB enhanced with new display
                   formats
NEWS 16   MAR 11   EPFULL backfile enhanced with additional full-text
                   applications and grants
NEWS 17   MAR 11   ESBIOBASE reloaded and enhanced
NEWS 18   MAR 20   CAS databases on STN enhanced with new super role
                   for nanomaterial substances
NEWS 19   MAR 23   CA/CAplus enhanced with more than 250,000 patent
                   equivalents from China
NEWS 20   MAR 30   IMSPATENTS reloaded and enhanced
NEWS 21   APR 03   CAS coverage of exemplified prophetic substances
                   enhanced
NEWS 22   APR 07   STN is raising the limits on saved answers
NEWS 23   APR 24   CA/CAplus now has more comprehensive patent assignee
                   information
NEWS 24   APR 26   USPATFULL and USPAT2 enhanced with patent
                   assignment/reassignment information
NEWS 25   APR 28   CAS patent authority coverage expanded
NEWS 26   APR 28   ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 27   APR 28   Limits doubled for structure searching in CAS
                   REGISTRY

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
             AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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=> ISCOMATRIX
L1        102 ISCOMATRIX

=> HCV
L2      45943 HCV

=> L1 and L2
L3          4 L1 AND L2

=> D L3 IBIB ABS 1-4

L3    ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2009 ACS on STN

| Full Text | Same References |
| --- | --- |

ACCESSION NUMBER:        2008:880662  CAPLUS
DOCUMENT NUMBER:         149:150269
TITLE:                   Induction of broad CD4+ and CD8+ T-cell responses and
                         cross-neutralizing antibodies against hepatitis C
                         virus by vaccination with Th1-adjuvanted polypeptides
                         followed by defective alphaviral particles expressing
                         envelope glycoproteins gpE1 and gpE2 and nonstructural
                         proteins 3, 4, and 5
AUTHOR(S):               Lin, Yinling; Kwon, Taewoo; Polo, John; Zhu, Yi-Fei;
                         Coates, Stephen; Crawford, Kevin; Dong, Christine;
                         Wininger, Mark; Hall, John; Selby, Mark; Coit, Doris;
                         Medina-Selby, Angelica; McCoin, Colin; Ng, Philip;
                         Drane, Debbie; Chien, David; Han, Jang; Vajdy,
                         Michael; Houghton, Michael
CORPORATE SOURCE:        Novartis Vaccine and Diagnostic, Inc., Emeryville, CA,
                         94608, USA
SOURCE:                  Journal of Virology (2008), 82(15), 7492-7503
                         CODEN: JOVIAM; ISSN: 0022-538X
PUBLISHER:               American Society for Microbiology
DOCUMENT TYPE:           Journal
LANGUAGE:                English
AB   Broad, multispecific CD4+ and CD8+ T-cell responses to the hepatitis C
     virus (HCV), as well as virus-cross-neutralizing antibodies, are assocd.
     with recovery from acute infection and may also be assocd. in chronic
     HCV patients with a favorable response to antiviral treatment.  In order
     to recapitulate all of these responses in an ideal vaccine regimen, we

have explored the use of recombinant **HCV** polypeptides combined with various Th1-type adjuvants and replication-defective alphaviral particles encoding **HCV** proteins in various prime/boost modalities in BALB/c mice. Defective chimeric alphaviral particles derived from the Sindbis and Venezuelan equine encephalitis viruses encoding either the **HCV** envelope glycoprotein gpE1/gpE2 heterodimer (E1E2) or nonstructural proteins 3, 4, and 5 (NS345) elicited strong CD8+ T-cell responses but low CD4+ T helper responses to these **HCV** gene products. In contrast, recombinant E1E2 glycoproteins adjuvanted with MF59 contg. a CpG oligonucleotide elicited strong CD4+ T helper responses but no CD8+ T-cell responses. A recombinant NS345 polyprotein also stimulated strong CD4+ T helper responses but no CD8+ T-cell responses when adjuvanted with **Iscomatrix** contg. CpG. Optimal elicitation of broad CD4+ and CD8+ T-cell responses to E1E2 and NS345 was obtained by first priming with Th1-adjuvanted proteins and then boosting with chimeric, defective alphaviruses expressing these **HCV** genes. In addn., this prime/boost regimen resulted in the induction of anti-E1E2 antibodies capable of cross-neutralizing heterologous **HCV** isolates in vitro. This vaccine formulation and regimen may therefore be optimal in humans for protection against this highly heterogeneous global pathogen.

L3    ANSWER 2 OF 4   CAPLUS   COPYRIGHT 2009 ACS on STN

Full  Citing
Text  References

ACCESSION NUMBER:          2006:943250  CAPLUS
DOCUMENT NUMBER:           146:106962
TITLE:                     The **ISCOMATRIX** adjuvant
AUTHOR(S):                 Drane, Debbie; Pearse, Martin J.
CORPORATE SOURCE:          CSL Limited, Parkville, Australia
SOURCE:                    Immunopotentiators in Modern Vaccines (2006), 191-215.
                           Editor(s): Schijns, Virgil E. J. C.; O'Hagan, Derek T.
                           Elsevier Inc.: Burlington, Mass.
                           CODEN: 69IKTO; ISBN: 978-0-12-088403-2
DOCUMENT TYPE:             Conference; General Review
LANGUAGE:                  English
AB   A review.  **ISCOMATRIX** adjuvant is essentially the same structure as the
     ISCOM vaccine but without the incorporated antigen. Antigens can be
     formulated with the **ISCOMATRIX** adjuvant to produce **ISCOMATRIX** vaccines
     which provide the same antigen presentation and immunomodulatory
     properties as ISCOM vaccines but much broader application. **ISCOMATRIX**
     vaccines are safe and well tolerated in humans with no vaccine-related
     serious adverse events or clin. significant lab. abnormalities reported.
     **ISCOMATRIX** vaccines are capable of inducing strong humoral responses
     with increases in the magnitude, speed, and longevity of the responses, as
     well as the capacity for antigen dose redn. when compared to other
     adjuvants such as aluminum. The properties of **ISCOMATRIX** vaccines make
     them viable candidates for the further development and registration of
     prophylactic and therapeutic human vaccines.
REFERENCE COUNT:           87    THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS
                           RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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Text  References

ACCESSION NUMBER:          2001:167132  CAPLUS
DOCUMENT NUMBER:           134:324389
TITLE:                     Characterization of hepatitis C virus core-specific
                           immune responses primed in rhesus macaques by a
                           nonclassical ISCOM vaccine
AUTHOR(S):                 Polakos, Noelle K.; Drane, Debbie; Cox, John; Ng,

                            Philip; Selby, Mark J.; Chien, David; O'Hagan, Derek
                            T.; Houghton, Michael; Paliard, Xavier

CORPORATE SOURCE:      Chiron Corp., Emeryville, CA, 94608, USA
SOURCE:                Journal of Immunology (2001), 166(5), 3589-3598
                            CODEN: JOIMA3; ISSN: 0022-1767
PUBLISHER:            American Association of Immunologists
DOCUMENT TYPE:        Journal
LANGUAGE:             English

AB   Current therapies for the treatment of hepatitis C virus (**HCV**) infection
    are only effective in a restricted no. of patients.  Cellular immune
    responses, particularly those mediated by CD8+ CTLs, are thought to play a
    role in the control of infection and the response to antiviral therapies.
    Because the Core protein is the most conserved **HCV** protein among
    genotypes, the authors evaluated the ability of a Core prototype vaccine
    to prime cellular immune responses in rhesus macaques.  Since there are
    serious concerns about using a genetic vaccine encoding for Core, this
    vaccine was a non-classical ISCOM formulation in which the Core protein
    was adsorbed onto (not entrapped within) the **ISCOMATRIX**, resulting in
    ~1-μm particulates (as opposed to 40 nm for classical ISCOM
    formulations).  The authors report that this Core-ISCOM prototype vaccine
    primed strong CD4+ and CD8+ T cell responses.  Using intracellular
    staining for cytokines, the authors show that in immunized animals
    0.30-0.71 and 0.32-2.21% of the circulating CD8+ and CD4+ T cells, resp.,
    were specific for naturally processed **HCV** Core peptides.  Furthermore,
    this vaccine elicited a Th0-type response and induced a high titer of Abs
    against Core and long-lived cellular immune responses.  Finally, the
    authors provide evidence that Core-ISCOM could serve as an adjuvant for
    the **HCV** envelope protein E1E2.  Thus, these data provide evidence that
    Core-ISCOM is effective at inducing cellular and humoral immune responses
    in nonhuman primates.
REFERENCE COUNT:         27      THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
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Full Text    Citing References

ACCESSION NUMBER:     2009:93260  BIOSIS
DOCUMENT NUMBER:      PREV200900093260
TITLE:                Induction of broad CD4(+) and CD8(+) T-cell responses and
                            cross-neutralizing antibodies against hepatitis C virus by
                            vaccination with Th1-adjuvanted polypeptides followed by
                            defective alphaviral particles expressing envelope
                            glycoproteins gpE1 and gpE2 and nonstructural proteins 3,
                            4, and 5.

AUTHOR(S):           Lin, Yinling [Reprint Author]; Kwon, Taewoo; Polo, John;
                            Zhu, Yi-Fei; Coates, Stephen; Crawford, Kevin; Dong,
                            Christine; Wininger, Mark; Hall, John; Selby, Mark; Coit,
                            Doris; Medina-Selby, Angelica; McCoin, Colin; Ng, Philip;
                            Drane, Debbie; Chien, David; Han, Jang; Vajdy, Michael;
                            Houghtont, Michael
CORPORATE SOURCE:     4 Captain Dr 411, Emeryville, CA 94608 USA
                            yinlilin918@yahoo.com
SOURCE:               Journal of Virology, (AUG 2008) Vol. 82, No. 15, pp.
                            7492-7503.
                            CODEN: JOVIAM. ISSN: 0022-538X.
DOCUMENT TYPE:        Article
LANGUAGE:             English
ENTRY DATE:           Entered STN: 28 Jan 2009
                            Last Updated on STN: 28 Jan 2009
AB   Broad, multispecific CD4(+) and CD8(+) T-cell responses to the hepatitis C

virus (**HCV**), as well as virus-cross-neutralizing antibodies, are associated with recovery from acute infection and may also be associated in chronic **HCV** patients with a favorable response to antiviral treatment.  In order to recapitulate all of these responses in an ideal vaccine regimen, we have explored the use of recombinant **HCV** polypeptides combined with various Th1-type adjuvants and replication-defective alphaviral particles encoding **HCV** proteins in various prime/boost modalities in BALB/c mice.  Defective chimeric alphaviral particles derived from the Sindbis and Venezuelan equine encephalitis viruses encoding either the **HCV** envelope glycoprotein gpE1/gpE2 heterodimer (E1E2) or nonstructural proteins 3, 4, and 5 (NS345) elicited strong CD8(+) T-cell responses but low CD4(+) T helper responses to these **HCV** gene products.  In contrast, recombinant E1E2 glycoproteins adjuvanted with MF59 containing a CpG oligonucleotide elicited strong CD4(+) T helper responses but no CD8(+) T-cell responses.  A recombinant NS345 polyprotein also stimulated strong CD4(+) T helper responses but no CD8(+) T-cell responses when adjuvanted with **Iscomatrix** containing CpG. Optimal elicitation of broad CD4(+) and CD8(+) T-cell responses to E1E2 and NS345 was obtained by first priming with Th1-adjuvanted proteins and then boosting with chimeric, defective alphaviruses expressing these **HCV** genes.  In addition, this prime/boost regimen resulted in the induction of anti-E1E2 antibodies capable of cross-neutralizing heterologous **HCV** isolates in vitro.  This vaccine formulation and regimen may therefore be optimal in humans for protection against this highly heterogeneous global pathogen.


=> electronic (w) interaction
L4        4290 ELECTRONIC (W) INTERACTION

=> electronic (w) association
L5           8 ELECTRONIC (W) ASSOCIATION

=> adjuvant
L6      118110 ADJUVANT

=> L6 and L2
L7         227 L6 AND L2

=> L4 and L7
L8           0 L4 AND L7

=> L7 and L5
L9           0 L7 AND L5

=> D L5 1B1B ABS 1-8

L5   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2009 ACS on STN

| Full | Citing |
| Text | References |

ACCESSION NUMBER:          2008:1295583  CAPLUS
TITLE:                     Automated patent office documentation
INVENTOR(S):               Zellner, Samuel N.
PATENT ASSIGNEE(S):        AT&T Intellectual Property I, L.P., USA
SOURCE:                    U.S.
                           CODEN: USXXAM
DOCUMENT TYPE:             Patent
LANGUAGE:                  English
FAMILY ACC. NUM. COUNT:    1
PATENT INFORMATION:

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   PATENT NO.          KIND   DATE      APPLICATION NO.        DATE
   ---------------     ----   --------  --------------------   --------
   US 7444589          B2     20081028  US 2004-26790          20041230
PRIORITY APPLN. INFO.:                  US 2004-26790          20041230
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AB   The present disclosure provides systems and methods for automated patent
     office documentation.  Some embodiments provide for analyzing electronic
     content such as an issued patent, application for patent, Patent and
     Trademark Office (PTO) office action, associated patent support data such
     as PTO information, and/or other reference materials, along with user
     input to identify references to external information, create an
     **electronic association** to the external information, and insert the
     **electronic association** into the electronic content.
REFERENCE COUNT:           37    THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS
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ACCESSION NUMBER:          2008:746167  CAPLUS
DOCUMENT NUMBER:           149:104371
TITLE:                     Synthesis and Self-Association Properties of
                           Functionalized C3-Symmetric
                           Hexakis(p-substituted-phenylethynyl)triindoles
AUTHOR(S):                 Garcia-Frutos, Eva M.; Gomez-Lor, Berta
CORPORATE SOURCE:          Instituto de Ciencia de Materiales de Madrid, CSIC,
                           Madrid, 28049, Spain
SOURCE:                    Journal of the American Chemical Society (2008),
                           130(28), 9173-9177
                           CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:                 American Chemical Society
DOCUMENT TYPE:             Journal
LANGUAGE:                  English
OTHER SOURCE(S):           CASREACT 149:104371
AB   A no. of differently substituted phenylethynyl triindoles has been
     synthesized by 6-fold Sonogashira coupling in a key step.  This new series
     of hexaalkynyl triindoles self-assoc. through arene-arene interactions in
     soln.  The electronic communication of the external substituents with the
     central electron-rich triindole core has been demonstrated by means of
     cyclic voltammetry and optical absorption.  A study of the effect of the
     electronic character of peripheral substituents on their self-assocn.
     behavior is presented in an effort to shed light on the nature of the
     π-stacking interactions.
REFERENCE COUNT:           44    THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
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L5   ANSWER 3 OF 8  CAPLUS  COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:          2007:1154432  CAPLUS
DOCUMENT NUMBER:           147:448160
TITLE:                     Gene analogue finder: a GRID solution for finding
                           functionally analogous gene products
AUTHOR(S):                 Tulipano, Angelica; Donvito, Giacinto; Licciulli,
                           Flavio; Maggi, Giorgio; Gisel, Andreas
CORPORATE SOURCE:          Dipartimento Interateneo di Fisica, Universita e
                           Politecnico di Bari, Bari, 70126, Italy
SOURCE:                    BMC Bioinformatics (2007), 8, No pp. given
                           CODEN: BBMIC4; ISSN: 1471-2105
                           URL: http://www.biomedcentral.com/content/pdf/1471-

2105-8-329.pdf

| | |
|---|---|
| PUBLISHER: | BioMed Central Ltd. |
| DOCUMENT TYPE: | Journal; (online computer file) |
| LANGUAGE: | English |

AB   To date more than 2,1 million gene products from more than 100000
     different species have been described specifying their function, the
     processes they are involved in and their cellular localization using a
     very well defined and structured vocabulary, the gene ontol. (GO).  Such
     vast, well defined knowledge opens the possibility of comparing gene
     products at the level of functionality, finding gene products which have a
     similar function or are involved in similar biol. processes without
     relying on the conventional sequence similarity approach.  Comparisons
     within such a large space of knowledge are highly data and computing
     intensive.  For this reason this project was based upon the use of the
     computational GRID, a technol. offering large computing and storage
     resources.  We have developed a tool, gEne analog fINdEr (ENGINE) that
     parallelizes the search process and distributes the calcn. and data over
     the computational GRID, splitting the process into many sub-processes and
     joining the calcn. and the data on the same machine and therefore
     completing the whole search in about 3 days instead of occupying one
     single machine for more than 5 CPU years.  The results of the functional
     comparison contain potential functional analogs for more than 79000 gene
     products from the most important species.  46% Of the analyzed gene
     products are well enough described for such an anal. to individuate
     functional analogs, such as well-known members of the same gene family, or
     gene products with similar functions which would never have been assocd.
     by std. methods.  ENGINE has produced a list of potential functionally
     analogous relations between gene products within and between species
     using, in place of the sequence, the gene description of the GO, thus
     demonstrating the potential of the GO.  However, the current limiting
     factor is the quality of the assocns. of many gene products from non-model
     organisms that often have **electronic assocns.**, since exptl.
     information is missing.  With future improvements of the GO, this limit
     will be reduced.  ENGINE will manifest its power when it is applied to the
     whole GODB of more than 2,1 million gene products from more than 100000
     organisms.  The data produced by this search is planned to be available as
     a supplement to the GO database as soon as we are able to provide regular
     updates.

| | | |
|---|---|---|
| REFERENCE COUNT: | 24 | THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS |
| | | RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT |

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Full  End
Text  References

| | |
|---|---|
| ACCESSION NUMBER: | 2004:300940  CAPLUS |
| DOCUMENT NUMBER: | 140:419575 |
| TITLE: | Single-Site Mutation and Secondary Structure |
| | Stability: An Isodesmic Reaction Approach. The Case of |
| | Unnatural Amino Acid Mutagenesis Ala→Lac |
| AUTHOR(S): | Cieplak, Andrzej Stanislaw; Suermeli, Nur Basak |
| CORPORATE SOURCE: | Department of Chemistry, Bilkent University, Bilkent, |
| | Ankara, 06800, Turk. |
| SOURCE: | Journal of Organic Chemistry (2004), 69(10), 3250-3261 |
| | CODEN: JOCEAH; ISSN: 0022-3263 |
| PUBLISHER: | American Chemical Society |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |

AB   A method is described to evaluate backbone interactions in proteins via
     computational unnatural amino acid mutagenesis.  Several N-acetyl
     polyalanyl amides (AcAnNH2) were optimized in the representative helical

(310-, 413-, and a "hybrid" κ-helix, n = 7, 9, 10, 14) and hairpin
(two- and three-stranded antiparallel β-sheets with type I turns
βααr, n = 6, 9, 10) conformations, and extended
conformers of N-acetyl polyalanyl methylamides (n = 2, 3) were used to
derive multistranded β-sheet fragments.  Subsequently, each residue
of every model structure was substituted, one at a time, with L-lactic
acid.  The resulting mutant structures were again optimized, and
group-transfer energies ΔEGT were obtained as heats of the isodesmic
reactions: AcAnNHR + AcOMe → AcAxLacAyNHR + AcNHMe (R = H, CH3).
These group-transfer energies correlate with the degree of charge
polarization of the substituted peptide linkages as measured by the
difference Δe in H and O Mulliken populations in HN-C:O and with the
H-bond distances in the "wild-type" structures.  A good correlation
obtains for the HF/3-21G and B3LYP/6-31G* group-transfer energies.  The
destabilization effects are interpreted in terms of loss of interstrand
and intrastrand H-bonds, decrease in Lewis basicity of the C:O group, and
O···O repulsion.  On the basis of several comparisons
of Ala → Lac ΔEGT's with heats of the NH → CH2
substitutions, the latter contribution is estd. (B3LYP/6-31G*) to range
between 1.5 and 2.4 kcal mol-1, a figure close to the recent exptl.
ΔΔG° value of 2.6 kcal mol-1 (McComas, C. C.; Crowley,
B. M.; Boger, D. L. J. Am. Chem. Soc. 2003, 125, 9314).  The partitioning
yields the following max. values of the **electronic assocn.** energy of
H-bonds in the examd. sample of model structures (B3LYP/6-31G* ests.):
310-helix De = -1.7 kcal mol-1, α-helix De = -3.8 kcal mol-1,
β-sheet De = -6.1 kcal mol-1.  The premise of exptl. evaluations of
the backbone backbone H-bonding that Ala → Lac substitution in
proteins is isosteric (e.g., Koh, J. T.; Cornish, V. W.; Schultz, P. G.
Biochem. 1997, 36, 11314) is often but not always corroborated.  Examn. of
the integrity of H-bonding pattern and φi, ψi distribution
identified several mutants with significant distortions of the "wild-type"
structure resulting inter alia from the transitions between i, i + 3 and
i, i + 4 H-bonding in helixes, obsd. previously in the crystallog. studies
of depsipeptides (Ohyama, T.; Oku, H.; Hiroki, A.; Maekawa, Y.; Yoshida,
M.; Katakai, R. Biopolymers 2000, 54, 375; Karle, I. L.; Das, C.; Balaram,
P. Biopolymers 2001, 59, 276).  Thus, the isodesmic reaction approach
provides a simple way to gauge how conformation of the polypeptide chain
and dimensions of the H-bonding network affect the strength of
backbone-backbone C:O···HN bonds.  The results
indicate that the stabilization provided by such interactions increases on
going from 310-helix to α-helix to β-sheet.

REFERENCE COUNT:          101   THERE ARE 101 CITED REFERENCES AVAILABLE FOR
                                THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
                                FORMAT

AB    Although the existence of Cα-H···O:C hydrogen
      bonds in protein structures recently has been established, little is known
      about their strength and, therefore, the relative importance of these
      interactions.  We have discovered that similar interactions occur in
      N,N-dimethylformamide dimers.  High level ab initio calcns.
      (MP2/aug-cc-pTZV) yield **electronic assocn.** energies (De) and assocn.
      enthalpies (ΔH298) for four dimer geometries.  These data provide a
      lower limit of De = -2.1 kcal mol-1 for the
      Cα-H···O:C hydrogen bond.  A linear correlation
      between C-H···O bond energies and gas-phase proton
      affinities is reported.  The gas-phase anion proton affinity of a peptide
      Cα-H hydrogen was calcd. (355 kcal mol-1) and used to est. values of
      De = -4.0 ± 0.5 kcal mol-1 and ΔH298 = -3.0 ± 0.5 kcal mol-1
      for the Cα-H···O:C hydrogen bond.  The
      magnitude of this interaction, roughly one-half the strength of the
      N-H···O:C hydrogen bond, suggests that
      Cα-H···O:C hydrogen bonding interactions
      represent a hitherto unrecognized, significant contribution in the detn.
      of protein conformation.
REFERENCE COUNT:           92      THERE ARE 92 CITED REFERENCES AVAILABLE FOR THIS
                                   RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


L5    ANSWER 6 OF 8  BIOSIS   COPYRIGHT (c) 2009 The Thomson Corporation   on STN

Full Text    Citing References

AB    Background: To date more than 2,1 million gene products from more than
      100000 different species have been described specifying their function,
      the processes they are involved in and their cellular localization using a
      very well defined and structured vocabulary, the gene ontology (GO).  Such
      vast, well defined knowledge opens the possibility of compare gene
      products at the level of functionality, finding gene products which have a
      similar function or are involved in similar biological processes without
      relying on the conventional sequence similarity approach.  Comparisons
      within such a large space of knowledge are highly data and computing
      intensive.  For this reason this project was based upon the use of the
      computational GRID, a technology offering large computing and storage
      resources.Results: We have developed a tool, GENe AnaloGue FINdEr (ENGINE)
      that parallelizes the search process and distributes the calculation and

data over the computational GRID, splitting the process into many
sub-processes and joining the calculation and the data on the same machine
and therefore completing the whole search in about 3 days instead of
occupying one single machine for more than 5 CPU years. The results of
the functional comparison contain potential functional analogues for more
than 79000 gene products from the most important species. 46% of the
analyzed gene products are well enough described for such an analysis to
individuate functional analogues, such as well-known members of the same
gene family, or gene products with similar functions which would never
have been associated by standard methods.Conclusion: ENGINE has produced a
list of potential functionally analogous relations between gene products
within and between species using, in place of the sequence, the gene
description of the GO, thus demonstrating the potential of the GO.
However, the current limiting factor is the quality of the associations of
many gene products from non-model organisms that often have **electronic
associations**, since experimental information is missing. With future
improvements of the GO, this limit will be reduced. ENGINE will manifest
its power when it is applied to the whole GODB of more than 2,1 million
gene products from more than 100000 organisms. The data produced by this
search is planed to be available as a supplement to the GO database as
soon as we are able to provide regular updates.

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AB   A method is described to evaluate backbone interactions in proteins via
     computational unnatural amino acid mutagenesis. Several N-acetyl
     polyalanyl amides (AcAnNH2) were optimized in the representative helical
     (310-, 413-, and a "hybrid" kappa-helix, n = 7, 9, 10, 14) and hairpin
     (two- and three-stranded antiparallel beta-sheets with type I turns
     betaalphaalphamember, n 6, 9, 10) conformations, and extended conformers
     of N-acetyl polyalanyl methylamides (n 2, 3) were used to derive
     multistranded beta-sheet fragments. Subsequently, each residue of every
     model structure was substituted, one at a time, with L-lactic acid. The
     resulting mutant structures were again optimized, and group-transfer
     energies DELTAEGT were obtained as heats of the isodesmic reactions:
     AcAnNHR + AcOMe fwdarw AcAxLacAyNHR + AcNHMe (R = H, CH3). These
     group-transfer energies correlate with the degree of charge polarization
     of the substituted peptide linkages as measured by the difference DELTAe
     in H and O Mulliken populations in HN-C=O and with the H-bond distances in
     the "wild-type" structures. A good correlation obtains for the HF/3-21G
     and B3LYP/6-31G* group-transfer energies. The destabilization effects are
     interpreted in terms of loss of interstrand and intrastrand H-bonds,
     decrease in Lewis basicity of the C=O group, and OcntdotcntdotcntdotO

repulsion.  On the basis of several comparisons of Ala fwdarw Lac
DELTAEGT'S with heats of the NH fwdarw CH2 substitutions, the latter
contribution is estimated (B3LYP/6-31G*) to range between 1.5 and 2.4 kcal
mol-1, a figure close to the recent experimental DELTADELTAGdegree value
of 2.6 kcal mol-1 (McComas, C.  C.; Crowley, B.  M.; Boger, D.  L.  J.
Am.  Chem.  Soc. 2003, 125, 9314).  The partitioning yields the following
maximum values of the **electronic association** energy of H-bonds in the
examined sample of model structures (B3LYP/6-31G* estimates): 310-helix De
= -1.7 kcal mol-1, alpha-helix De = -3.8 kcal mol-1, beta-sheet De = -6.1
kcal mol-1.  The premise of experimental evaluations of the
backbone-backbone H-bonding that Ala fwdarw Lac substitution in proteins
is isosteric (e.g., Koh, J.  T.; Cornish, V.  W.; Schultz, P.  G.
Biochemistry 1997, 36, 11314) is often but not always corroborated.
Examination of the integrity of H-bonding pattern and phii, psii
distribution identified several mutants with significant distortions of
the "wild-type" structure resulting inter alia from the transitions
between i, i + 3 and i, i + 4 H-bonding in helices, observed previously in
the crystallographic studies of depsipeptides (Ohyama, T.; Oku, H.;
Hiroki, A.; Maekawa, Y.; Yoshida, M.; Katakai, R.  Biopolymers 2000, 54,
375; Karle, I.  L.; Das, C.; Balaram, P.  Biopolymers 2001, 59, 276).
Thus, the isodesmic reaction approach provides a simple way to gauge how
conformation of the polypeptide chain and dimensions of the H-bonding
network affect the strength of backbone-backbone C=OcntdotcntdotcntdotHN
bonds.  The results indicate that the stabilization provided by such
interactions increases on going from 310-helix to aalphahelix to
beta-sheet.

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TITLE:               DNA protection from iron-adriamycin-induced oxidative
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AUTHOR(S):           Musich, Phillip R. [Reprint author]; Campbell, Sharon E.
                     [Reprint author]; Chua, Balvin H. [Reprint author]
CORPORATE SOURCE:    East Tennessee State University, College of Medicine,
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SOURCE:              FASEB Journal, (March 7, 2001) Vol. 15, No. 4, pp. A512.
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DOCUMENT TYPE:       Conference; (Meeting)
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LANGUAGE:            English
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AB   Adriamycin (ADR), is an effective anti-cancer agent.  It is an
     anthracycline drug with a fused ring system that is planar, hydrophobic
     and electron rich, features which allow DNA intercalation.  Its
     anti-neoplastic effectiveness stems from its ability to intercalate into
     DNA and inhibit topoisomerase.  ADR also chelates Fe+3 ions and this
     complex (FeADR (1:2)) oxidatively cleaves DNA via a free radical
     interaction.  As shown by Nohl et al. (1998, Z.  Naturforsch,
     53c:279-285), enzymes associated specifically with heart mitochondria,
     increase.  ADR free radical formation explaining why it is selectively
     cardiotoxic.  Pretreatment of mice with the neural hormone melatonin
     eliminates the cardiotoxic effect of ADR therapy without reducing the

drug's antitumor effect (Liu et al. 2000, FASEB J. 14:113.9).  The purpose
of this study is to analyze the mechanistic features of DNA damage by an
Fe+3 ADR (1:2) complex (FeADR) and how melatonin ameliorates this damage.
FeADR + glutathione (GSH) cleaves DNA; this oxidative cleavage does not
occur with ADR +/- GSH or with FeADR in the absence of GSH.  Melatonin
reduces this oxidative DNA cleavage by 67%.  Mechanistic studies using a
supercoiled-to-nicked-circular-conversion assay in conjunction with
spectroscopic analyses reveal that: 1) FeADR + GSH forms a reactive
intermediate. 2) Melatonin protects the DNA from cleavage by this reactive
intermediate. 3) GSH reduction of FeADR diminishes the **electronic
association** between the ADR and iron in the complex. 4) FeADR as well as
ADR intercalates into DNA. 5) The intercalation of FeADR into DNA alters
the rate of oxidative DNA damage. 6) Melatonin also binds to DNA but not
by intercalation.  These experiments indicate that the cardioprotective
effect of melatonin in ADR therapy may stem from melatonin's interaction
with a reactive intermediate of FeADR + GSH, and/or a direct DNA
interaction.  Mechanistic features of this protection by melatonin may
involve melatonin-iron interactions or effects on DNA that modify the
FeADR intercalation.

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